4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of ammonia are presented in Table 4-1. These data are for ammonia in its pure gaseous state (i.e., anhydrous ammonia). Ammonia is also commercially and commonly available as an aqueous solution; the most common commercial formulation is 28–30% NH_3 (Weast et al. 1988). At this concentration, ammonia forms a nearly saturated solution in water. Data on ammonia in aqueous solution, ammonium hydroxide, and ammonium ion are also included in Table 4-1 where appropriate.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

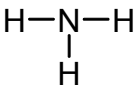
Ammonium hydroxide is a weak base that is partially ionized in water according to the equilibrium:

$$NH_3 + H_20 \quad o \quad [NH_4OH] \quad o \quad NH_4^+ + OH^-$$

The dissociation constant, K_b, is $1.774x10^5$ at 25 °C (pK_b is 4.751) and increases slightly with increasing temperature (Weast et al. 1988). At pH 9.25 half of the ammonia will be un-ionized (NH_3) and half will be ionized (NH_4^+). At pH 8.25 and 7.25, 90, and 99% of the ammonia will be ionized, respectively. Therefore, at most environmentally significant pHs, ammonia will be largely ionized; the fraction of un-ionized ammonia will become increasingly more important at pHs above 7. As a result, many physical and chemical properties will be a function of pH. For example, the solubility of ammonia in water will increase with decreasing pH. The volatility of ammonia increases with increasing pH; therefore, it volatilizes freely from solution at high pH values. Ammonium salts such as chloride, nitrate, and sulfate are strongly dissociated and very soluble in water (Weast et al. 1988); therefore, changes in pH will not normally result in the formation of ammonium precipitates.

The physical and chemical properties of ammonia are presented in Table 4-2. Also included are some chemical and physical properties of ammonia in solution. Ammonia in solution is widely available, and it is often referred to as ammonium hydroxide and has been also historically referred to as “spirit of hartshorn” (Windholz 1983).

Table 4-1. Chemical Identity of Ammonia

Characteristic	Information	Reference
Chemical name	Ammonia	
Synonym(s)	Anhydrous ammonia, AM-FOL, Ammonia gas, Liquid ammonia, Nitro-sil, R 717, Spirit of hartshorn	EPA 1987a; Windholz 1983
Registered trade name(s)	No data	
Chemical formula	NH_3	
Chemical structure		
Identification numbers:		
CAS Registry	7664-41-7	HSDB 2003
NIOSH RTECS	B00875000	NIOSH 2002a
anhydrous ammonia	B00875000	
aqueous solution	B00875000	
aqua ammonia	B00875000	
EPA Hazardous Waste	No data	
OHM/TADS	7216584	OHM-TADS 1988
DOT/UN/NA/IMCO shipping		
anhydrous	UN 1005	NIOSH 2002a
solution (10–35%)	UN 2672	
solution (35–50%)	UN 2073	
solution (>50%)	UN 1005	
HSDB	162	HSDB 2003
NCI	No data	

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Physical and Chemical Properties of Ammonia

Property	Value	Reference
Molecular weight	17.03	LeBlanc et al. 1978
Color	Colorless	LeBlanc et al. 1978
Physical state	Gas at room temperature	LeBlanc et al. 1978
Melting point	-77.7 °C	LeBlanc et al. 1978
Boiling point	-33.35 °C	LeBlanc et al. 1978
Density:		
Gas	0.7710 g/L	Weast et al. 1988
Aqueous solution (28%)	0.89801 (20 °C) g/L	Windholz 1983
Liquid	0.6818 g/L (-33.35 °C, 1 atm)	Windholz 1983
Vapor density	0.5967 (air=1)	Windholz 1983
Specific gravity (25 °C)	0.747 g/L	Lide 1998
Odor	Sharp, intensely irritating	Sax and Lewis 1987
Odor threshold:		
Air	25 ppm (18 mg/m^3)	Amoore and Hautala 1983
	48 ppm (34 mg/m^3)	Leonardos et al. 1969
	53 ppm (38 mg/m^3)	Budavari et al. 1996
Water	1.5 ppm	Amoore and Hautala 1983
pKa	9.25 (25°C)	Lide 1998
Solubility:		
Water		
at 0 °C	42.8% (w/w)	LeBlanc et al. 1978
	47% (w/w)	Budavari et al. 1996
at 15 °C	38% (w/w)	Budavari et al. 1996
at 20 °C	33.1% (w/w)	LeBlanc et al. 1978
	34% (w/w)	Budavari et al. 1996
at 25 °C	34% (w/w)	LeBlanc et al. 1978
	31% (w/w)	Budavari et al. 1996
at 30 °C	28% (w/w)	Budavari et al. 1996
at 50 °C	18% (w/w)	Budavari et al. 1996
Organic solvent(s)		
at 0 °C	20% (w/w) in absolute ethanol	Budavari et al. 1996
at 25 °C	10% (w/w) in absolute ethanol	Budavari et al. 1996
	16% (w/w) in methanol	Budavari et al. 1996
	Soluble in chloroform and ether	Budavari et al. 1996
Partition coefficients:		
Log K_{ow}	0.23 (estimated)	EPIWIN 2000

Table 4-2. Physical and Chemical Properties of Ammonia

Property	Value	Reference
Log K_{oc}	1.155 (estimated)	EPIWIN 2000
Vapor pressure:		
Anhydrous NH_3	8.5 atm (20 °C)	Sax and Lewis 1987
	10.2 atm (25 °C)	Daubert and Danner 1989
Aqueous NH_3 (28%)	2.9 atm (25 °C)	Daubert and Danner 1989
Henry's law constant	1.6×10^{-5} atm-m^3/mol (25 °C)	Betterton 1992
	7.3×10^{-6} atm-m^3/mol (pH 7, 23.4 °C)[a]	Ayers et al. 1985
	1.60×10^{-5} atm-m^3/mol (25 °C)[b]	Yoo et al. 1986
	5.01×10^{-6} atm-m^3/mol (5 °C)	Brimblecombe and Dawson 1984
Autoignition temperature	650 °C	LeBlanc et al. 1978
Flashpoint	Not available	
Flammability limits in air	16–25%	LeBlanc et al. 1978
Conversion factors		
ppm (v/v) to mg/m^3 in air (20 °C)	1 ppm (v/v) = 0.707 mg/m^3	Verschueren 1983
mg/m^3 to ppm (v/v) in air (20 °C)	1 mg/m^3 = 1.414 ppm (v/v)	
pH in water	11.6 (1 N)	Windholz 1983
	11.1 (0.1 N)	
	10.6 (0.01 N)	
Explosive limits	Not available	

[a]Unitless constant extrapolated from cited data.
[b]Unconverted value of 0.0168 kg-atm/mol was calculated from equation in citation.

pKa = The dissociation constant of the conjugate acid